

1,1,2,2-Tetrafluoro-2-(1,1,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
104729-49-9 | DTXSID40446988

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.15×10^{-15} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.53×10^{-1}

Confidence level: 4.78×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Perfluorotributylamine

Measured: 6.00×10^{-17}

Predicted: 1.14×10^{-16}

Image not found

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-

Measured: 7.20×10^{-15}

Predicted: 1.32×10^{-14}

Image not found

Perfluorotriethylamine

Measured: 6.00×10^{-16}

Predicted: 6.45×10^{-16}

Image not found

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane

Measured: 7.50×10^{-14}

Predicted: 3.74×10^{-14}